# Population dynamics and rare events

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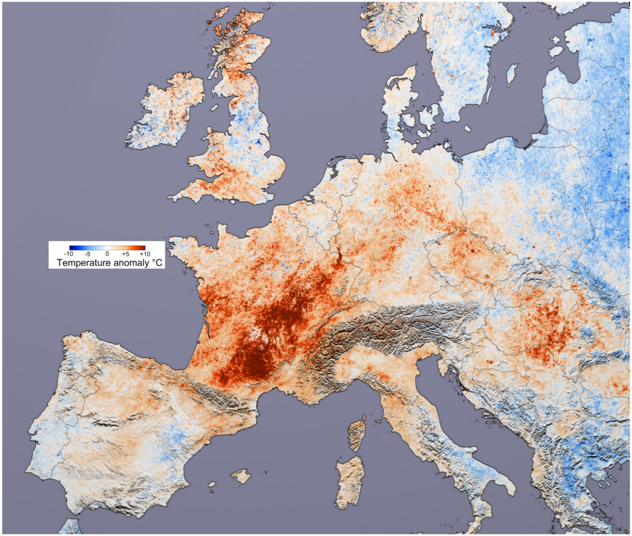
# Why studying rare events?




2003 heat wave, Europe [Terra MODIS]

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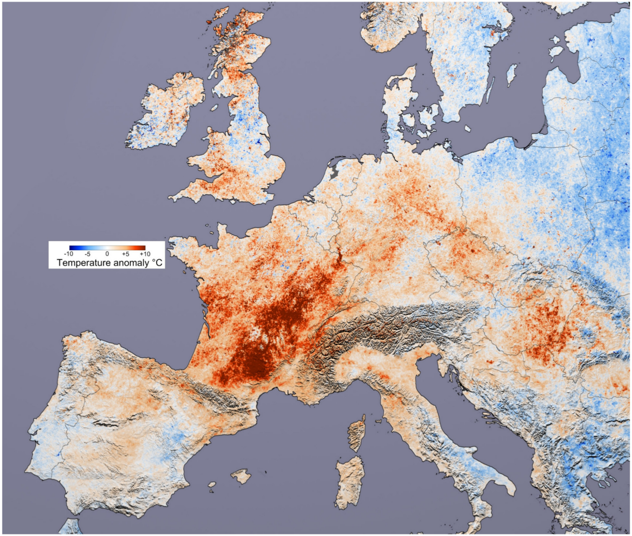


[Anomaly for **1-month** average] 2003 heat wave, Europe [Terra MODIS]

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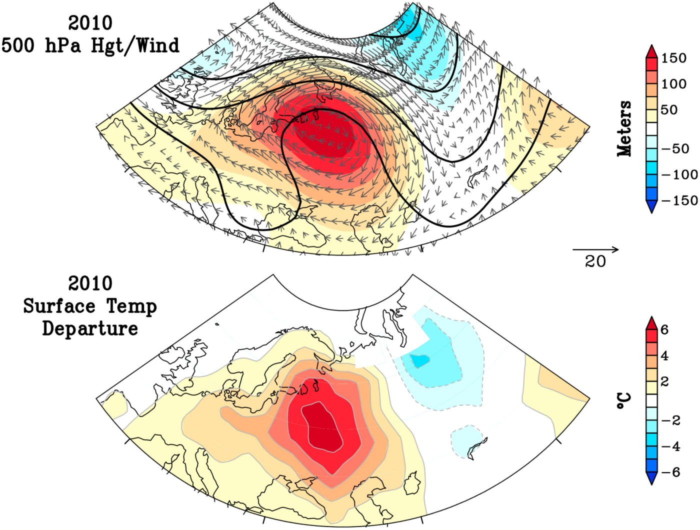


2010 heat wave in Western Russia [Dole *et al.*, 2011]

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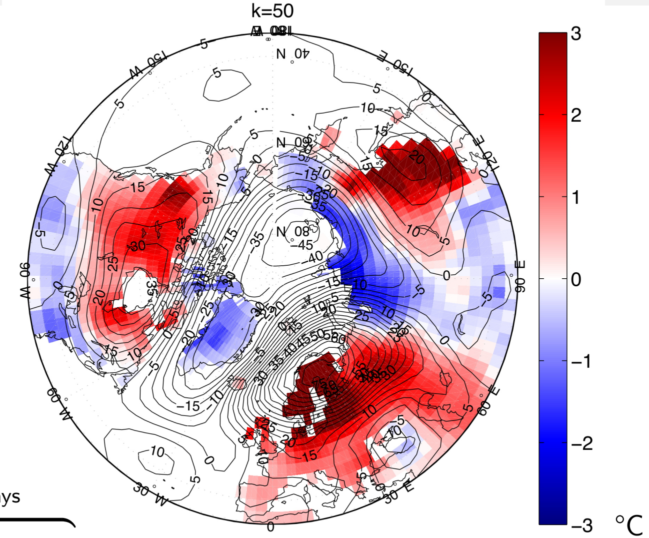


$$\overbrace{\frac{1}{t_{\max}}\int_0^{}dt\,\Delta T(t)}^{t=40\text{ days}}$$

« Teleconnection patterns » [Bouchet *et al.*]

# How to study rare events?

Questions for physicists and mathematicians:

- Probability and **dynamics** of rare events?
- How to **sample** these in numerical modelisation?
- Numerical **tools** and methods to understand their **formation**?

# Outline

- **Introduction**
- **Tools and algorithm**:
  - Large deviation functions
  - Ingredient 1/2: population dynamics
  - Ingredient 2/2: change of ensemble
- **Use, extensions and limitations of population dynamics**:
  - Different averages
  - Feedback method
  - Finite-time and finite-population scalings
- **Open questions**

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# Time-extensive observable on a time window $[0, t_f]$

- Climate dynamics:

$$\int_0^{t_f} dt \;\; \text{temperature}(t)$$

- Fluctuating thermodynamics:

$$\text{work} \;=\; \int_0^{t_f} dt \;\; \textbf{force}(t) \cdot \textbf{velocity}(t)$$

- Road traffic:

$$\#\{\text{cars passing through a gate}\}$$

- Molecular transport:

$$\#\{\text{steps of a motor on a filament}\}$$

- Lattice gases in 1d:

$$\text{“current”} \;=\; \#\{\text{jumps to the right}\} - \{\text{jumps to the left}\}$$
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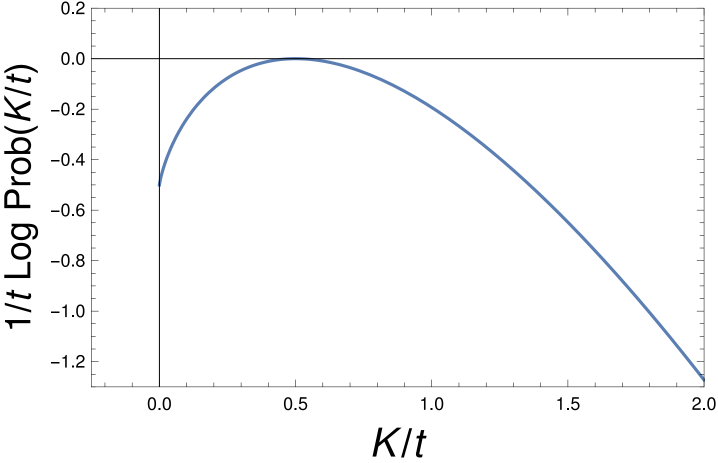
# Distribution of a time-extensive observable $K$ on $[0, t]$




$\mathrm{Prob}[K, t] \sim e^{t\,\varphi(K/t)}$ as $t \to \infty$ $\varphi(k)$ = large deviation function

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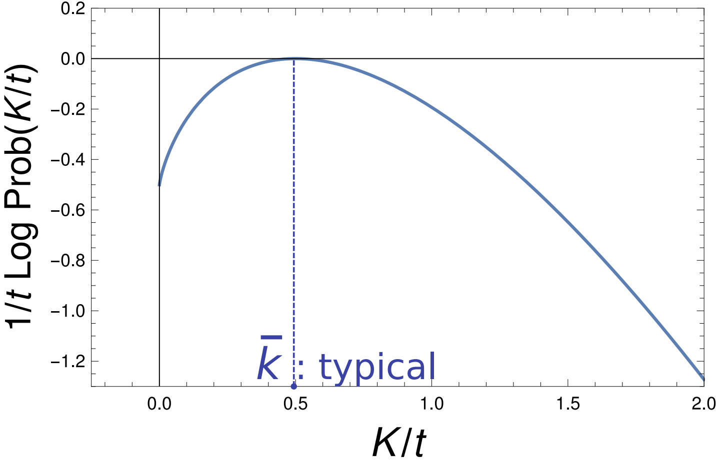


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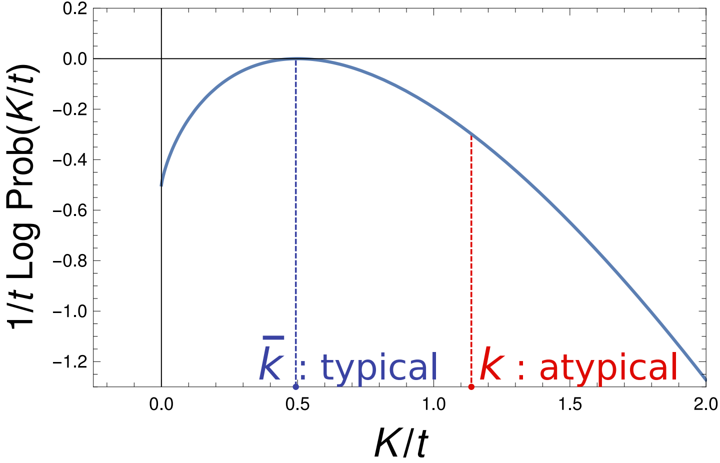


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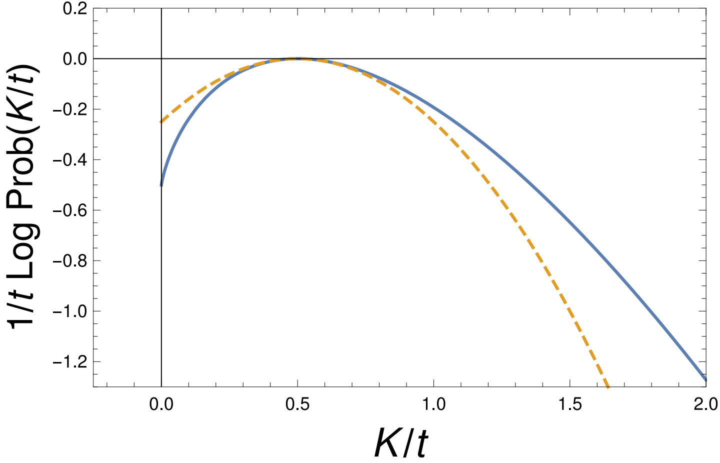


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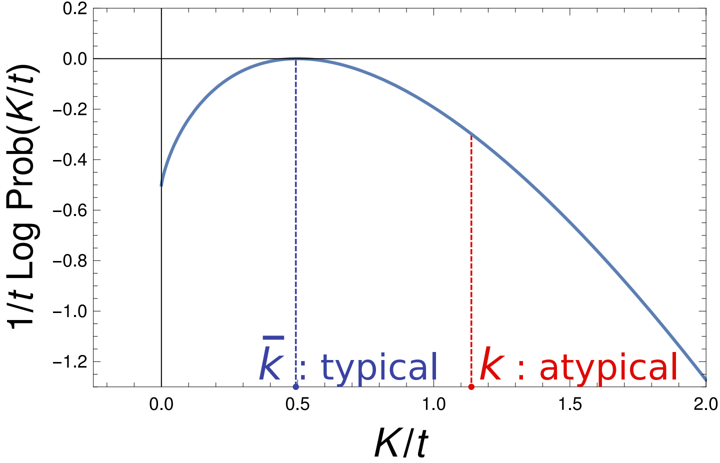
quadratic approx. $\varphi(k) = \frac{(k-\bar{k})^2}{2\sigma^2} + \dots$ $\leftrightarrow$ Gaussian fluctuations

# Aim: modify dynamics to make atypical values $k$ typical




Original dynamics: $\bar{k}$ is typical and $k$ atypical
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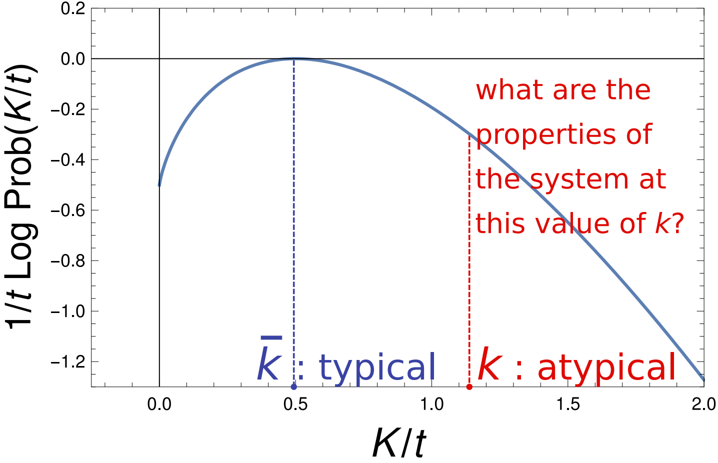


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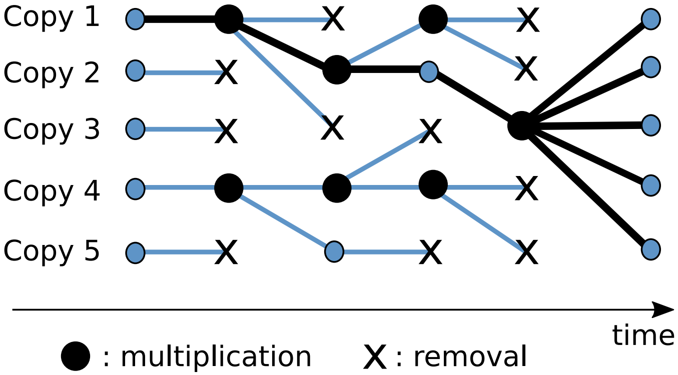


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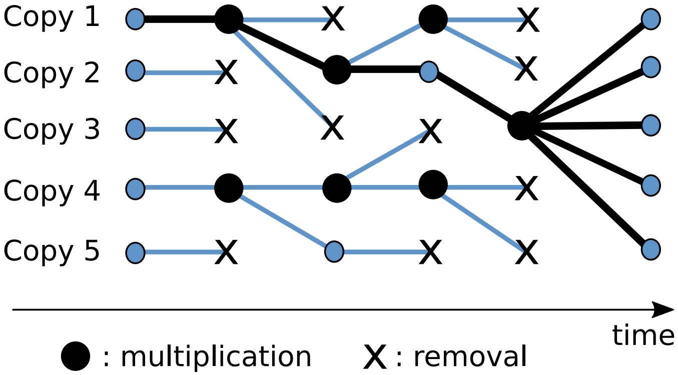


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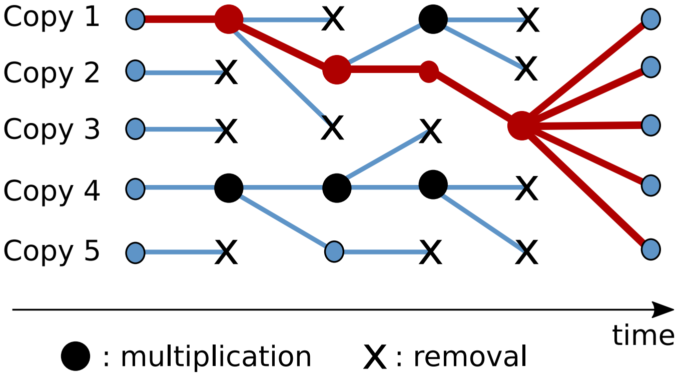


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**Selection rules** favor the normally atypical value of $k$
$\rightarrow$ **typical** population trajectories sample trajectories at $K/t = k$

# Ingredient 2/2: dynamical change of ensemble @$t \to \infty$

Consider an observable $\mathcal{O}[\text{trajectory}]$.

$$\underbrace{\frac{\big\langle \mathcal{O}[\text{traj.}]\,\delta\big(\tfrac{1}{t}K[\text{traj.}] - k\big)\big\rangle}{\big\langle \delta\big(\tfrac{1}{t}K[\text{traj.}] - k\big)\big\rangle}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{with atypical } k = K/t}}$$

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For $s$ and $k$ suitably "conjugated".

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**Next goal: show that** $\quad \ldots = \underbrace{\left\langle \mathcal{O}[\text{traj.}]\right\rangle_{\text{population dynamics}}}_{\substack{\text{average of } \mathcal{O} \text{ for trajectories} \\ \text{in fixed-size population} \\ \text{dynamics}}}$

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For $s$ and $k$ suitably “conjugated”.

Analogy: $k \equiv$ energy/volume; $s \equiv$ inverse temperature $\beta$

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Fixed $k = K/t \quad \Longleftrightarrow \quad$ bias by $e^{-sK}$

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Maximum reached for $k$ conjugated to $s$

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**Remaining question:** how to represent $e^{-sK}$ by pop. dynamics?

# $s$-modified dynamics (for jump processes)

- Markov processes: Configs. $\mathcal{C}$, jump rates $W(\mathcal{C} \to \mathcal{C}')$

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C}, t)}_{\text{loss term}} \Big\}$$

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## $s$-modified dynamics $\qquad K = k_{\mathcal{C}_0\mathcal{C}_1} + k_{\mathcal{C}_1\mathcal{C}_2} + \dots$

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# Numerical method [JB Anderson; D Aldous; P Grassberger; P Del Moral; ...]

## Evaluation of large deviation functions [*à la* “Diffusion Monte-Carlo”]

$$\sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t) = \left\langle \mathrm{e}^{-s\,K} \right\rangle \sim \mathrm{e}^{t\,\psi(s)} \qquad (\psi(s){=}\text{CGF}{=}\text{max eigenv. } \mathbb{W}_s)$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: VL, Tailleur [JSTAT P03004 (2007)]

## Cloning dynamics

$$\partial_t \hat{P}(\mathcal{C}, s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s) - r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C}) \hat{P}(\mathcal{C}, s)}_{\text{cloning term}}$$

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**How to take into account loss/gain of probability?**

- handle a large number $N_c$ of copies of the system
- implement a selection rule: on a time interval $\Delta t$
  a copy in config $\mathcal{C}$ is replaced by $Y = e^{\Delta t\, \delta r_s(\mathcal{C})}$ copies
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

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$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

**How to take into account loss/gain of probability?**

- handle a large number $N_c$ of copies of the system
- implement a selection rule: on a time interval $\Delta t$
  a copy in config $\mathcal{C}$ is replaced by $Y = \lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\varepsilon \sim [0,1]$
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

CGF estimator: $\psi(s) = \langle \Psi(s) \rangle$ with $\Psi(s) = \log \underbrace{\prod_t \frac{N_c + Y_t - 1}{N_c}}_{\text{reconstituted population size}}$

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## Biological interpretation

- copy in configuration $\mathcal{C}$ $\equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s$ $\equiv$ **mutations**
- cloning at rates $\delta r_s$ $\equiv$ **selection** rendering typical the rare histories

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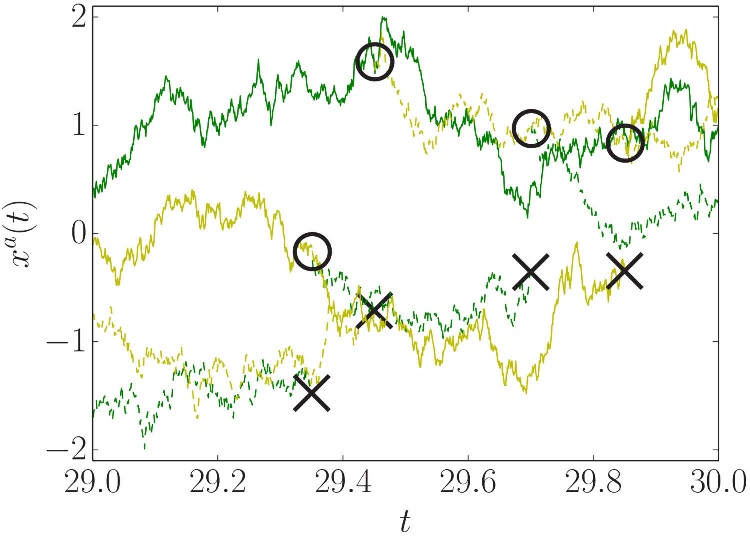
## Generic idea

- **Different dynamics can share equivalent statistical properties.**
- Constrained trajectories (fixed atypical $k = K/t$) $\equiv$ pop. dynamics

# An example: $4$ copies, $1$ degree of freedom $\mathcal{C} = x \in \mathbb{R}$



# How to perform averages? (i) [spectral analysis]

⋆ Final-time distribution $p_{\text{end}}(\mathcal{C})$: *proportion* of copies in $\mathcal{C}$ at $t$

$$\langle N_{\text{nc}}(t)\rangle_s$$

$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s}$$

[$N_{\text{nc}}$ = number of copies in non-constant population dynamics]

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$$\mathbb{W}_s|R\rangle = \psi(s)|R\rangle$$

$$\langle L|\mathbb{W}_s = \psi(s)\langle L|$$

$$[\quad \langle L| = \langle -| \ @\, s=0 \quad ]$$

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$$\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle \qquad \mathbb{W}_s |R\rangle = \psi(s) |R\rangle$$

$$e^{t\mathbb{W}_s} \underset{t\to\infty}{\sim} e^{t\psi(s)} |R\rangle\langle L| \qquad \langle L| \mathbb{W}_s = \psi(s) \langle L|$$

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$$\langle N_{\text{nc}}(t)\rangle_s = \langle -|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle L|P_{\text{i}}\rangle N_0$$

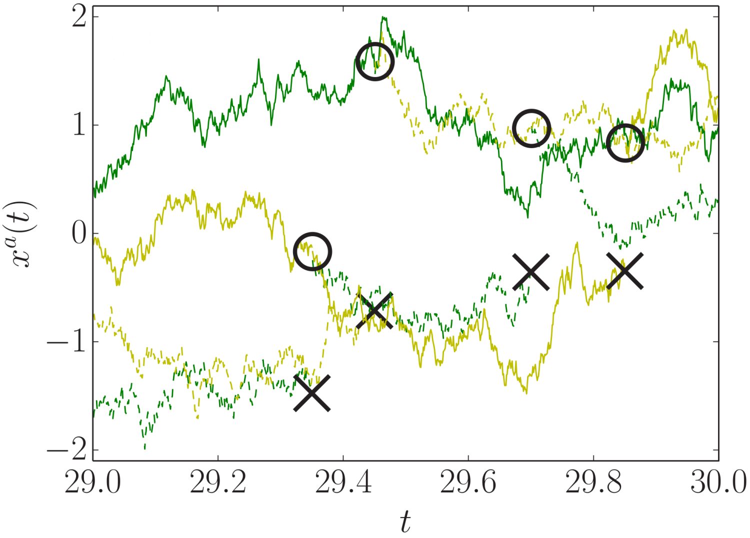
$$\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s = \langle \mathcal{C}|e^{t\mathbb{W}_s}|P_{\text{i}}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle \mathcal{C}|R\rangle\langle L|P_{\text{i}}\rangle N_0$$

$$p_{\text{end}}(\mathcal{C},t) = \frac{\langle N_{\text{nc}}(\mathcal{C},t)\rangle_s}{\langle N_{\text{nc}}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle \mathcal{C}|R\rangle \equiv p_{\text{end}}(\mathcal{C})$$

[$N_{\text{nc}}$ = number of copies in non-constant population dynamics]

**Final-time** distribution $p_{\text{end}}(\mathcal{C})$ governed by **right** eigenvector.

# An example: $4$ copies, $1$ degree of freedom $\mathcal{C} = x \in \mathbb{R}$



# How to perform averages? (ii) Intermediate times

$$\partial_t |\hat{P}\rangle = \mathbb{W}_s |\hat{P}\rangle \qquad \mathbb{W}_s |R\rangle = \psi(s)|R\rangle$$

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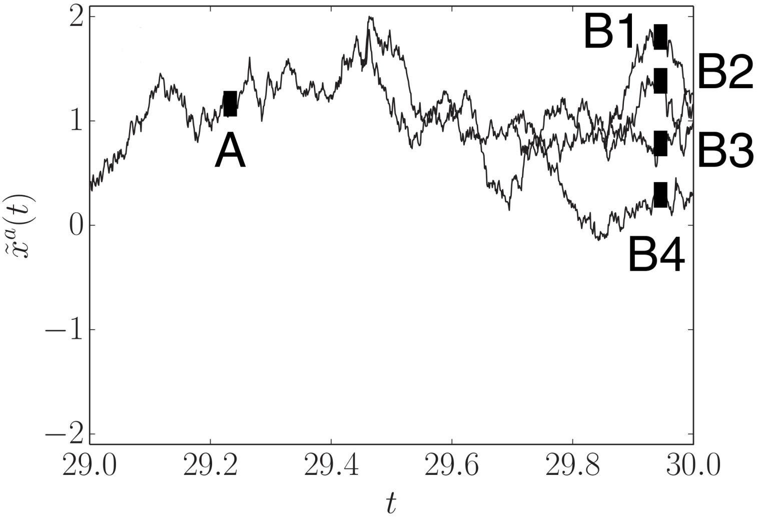
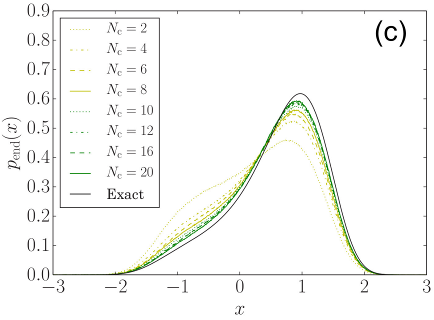
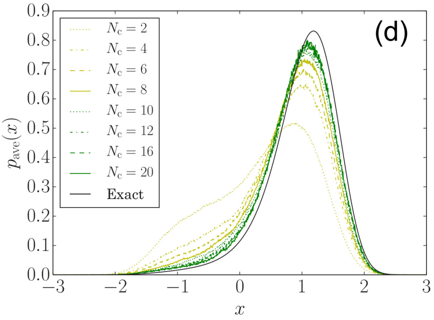



Huge sampling issue

# Example distributions for a simple Langevin dynamics



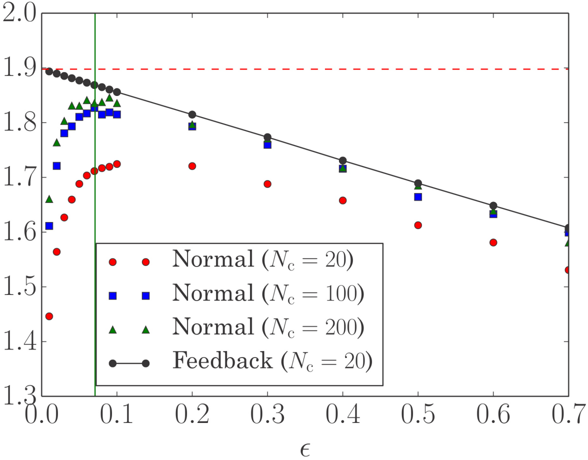




final-time: $p_{\mathrm{end}}(x)$
$(= R(x))$

intermediate-time: $p_{\mathrm{ave}}(x)$
$(= R(x)L(x))$

# The small-noise crisis: systematic errors grow as $\epsilon \to 0$

CGF as a function of the noise amplitude $\epsilon$:




Cause: as $\epsilon \to 0$, $p_{\text{ave}}(x)$ & $p_{\text{end}}(x)$ $\to$ sharply peaked at *different points*

*i.e.* the clones do not sample correctly the phase space

# The feedback method

# How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between $p_{\text{ave}}$ and $p_{\text{end}}$
- Constructed as **[Different dynamics can share ≡ statistical properties.]**

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

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- Issue: determining $L$ is difficult
- Solution: evaluate $L$ as $L_{\mathrm{test}}$ on the fly **[feedback]** and simulate

$$\mathbb{W}_s^{\mathrm{test}} = L_{\mathrm{test}} \mathbb{W}_s L_{\mathrm{test}}^{-1} \qquad \text{(induces \textit{\textbf{effective forces}})}$$

- **Iterate.** [For any $L_{\mathrm{test}}$, the simulation is in principle correct.]

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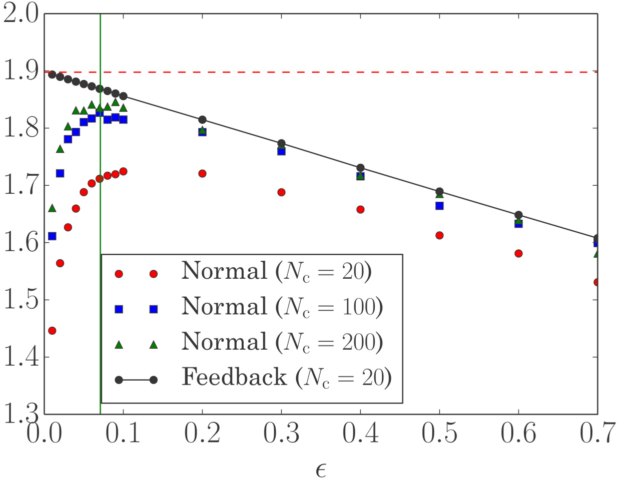
Similar in spirit to **multi-canonical** (*e.g.* Wang–Landau) approaches in static thermodynamics. [Here, one flattens the left-eigenvector of $\mathbb{W}_s^{\text{test}}$.]

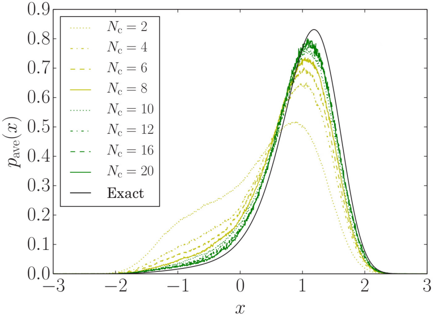
# Improvement of the small-noise crisis (i.i)

CGF as a function of the noise amplitude $\epsilon$:

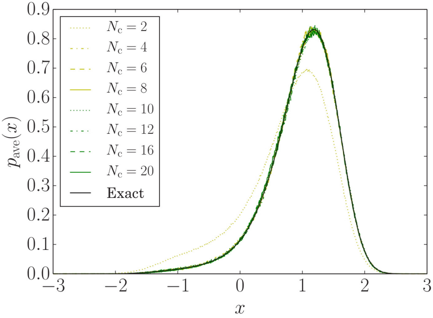



Physical insight: probability loss transformed into *effective forces*.

# Improvement of the small-noise crisis (i.ii)



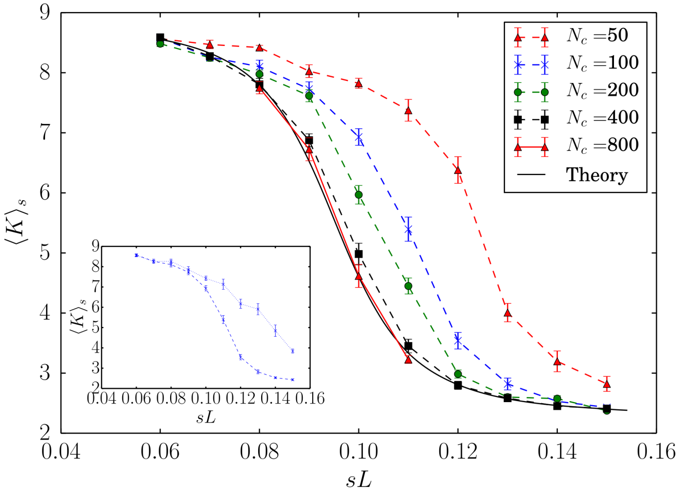

**Without feedback**




**With feedback**

Much more efficient evaluation of the biased distribution.
Even for a very crude (polynomial) approximation of the effective force.

# Improvement of the small-noise crisis (ii)

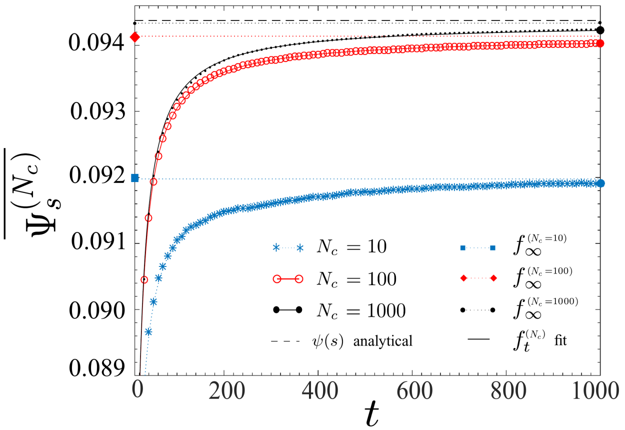



Interacting system in 1D.

Effective force: 1-, 2-, 3- body interactions only [also crude approx.].

# Finite-time and -population effects

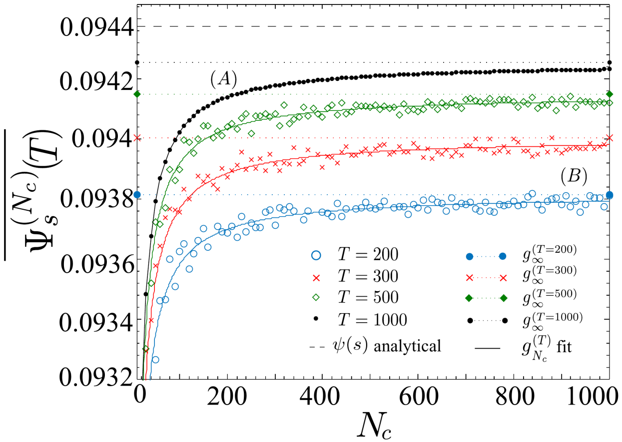
# Finite-time scaling [fixed population $N_c$]




Estimator converges in $1/t$ to its infinite-time limit

Understanding: the estimator is an additive observable of the pop. dyn.

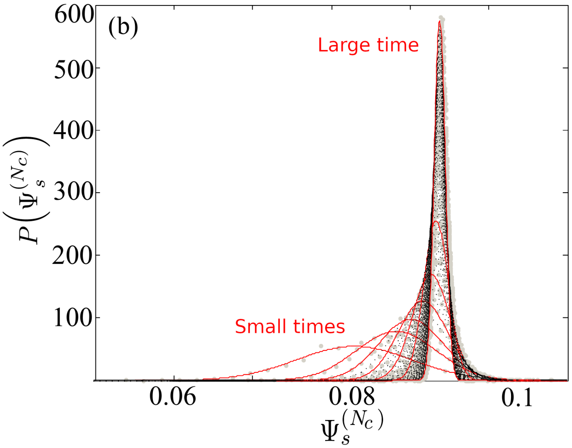
# Finite-$N_c$ scaling **[fixed time]**




Estimator converges in $1/N_c$ to its infinite-population limit

Understanding: large $N_c$ expansion, small-noise description

# Distribution of the CGF estimator **[fixed population $N_c$]**




In the numerics: $\approx$ Gaussian when finite-$N_c$ scaling is $O(1/N_c)$
A way to check why one is / is not in that regime

# Summary and open questions (1)

**Feedback method** [with F Bouchet, R Jack, T Nemoto]

- Sampling problem (depletion of ancestors)
- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

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## Feedback method [with F Bouchet, R Jack, T Nemoto]

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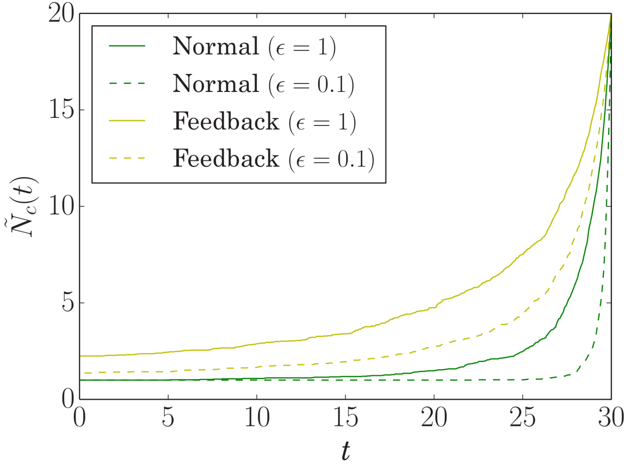
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

## Finite-population effects [with E Guevara, T Nemoto]

- Quantitative finite-$N_{\text{clones}}$ scaling $\rightarrow$ interpolation method
- Initial transient regime due to small population
- Analogy with biology: many small islands *vs.* few large islands?
- Question: effective forces $\leftarrow$ selection?

# Open questions (2): why is the feedback working?

Improvement of the depletion-of-ancestors problem:




Dashed line: lower noise Continuous line: higher noise

# Open questions (3)

## Finite-population and -time scalings

- Anomalous fluctuations (invalid $1/N_c$ asymptotics)
- Correct description of the meta-dynamics?
- Finite-$N_c$ and -$t$ scaling **with feedback**
- Phase transition in the distribution of the CGF estimator?

# Thank you for your attention!

**References**:


- ⋆ *Population dynamics method with a multi-canonical feedback control*
  Takahiro Nemoto, Freddy Bouchet, Robert L. Jack and Vivien Lecomte
  PRE **93** 062123 (2016)
- ⋆ *Finite-time and finite-size scalings in the evaluation of large deviation functions: Analytical study using a birth-death process*
  Takahiro Nemoto, Esteban Guevara Hidalgo and Vivien Lecomte
  PRE **95** 012102 (2017)
- ⋆ *Finite-size scaling of a first-order dynamical phase transition: adaptive population dynamics and effective model*
  Takahiro Nemoto, Robert L. Jack and Vivien Lecomte
  PRL **118** 115702 (2017)
- ⋆ *Finite-time and finite-size scalings in the evaluation of large deviation functions: Numerical approach in continuous time*
  Esteban Guevara Hidalgo, Takahiro Nemoto and Vivien Lecomte
  PRE **95** 062134 (2017)

# Supplementary material

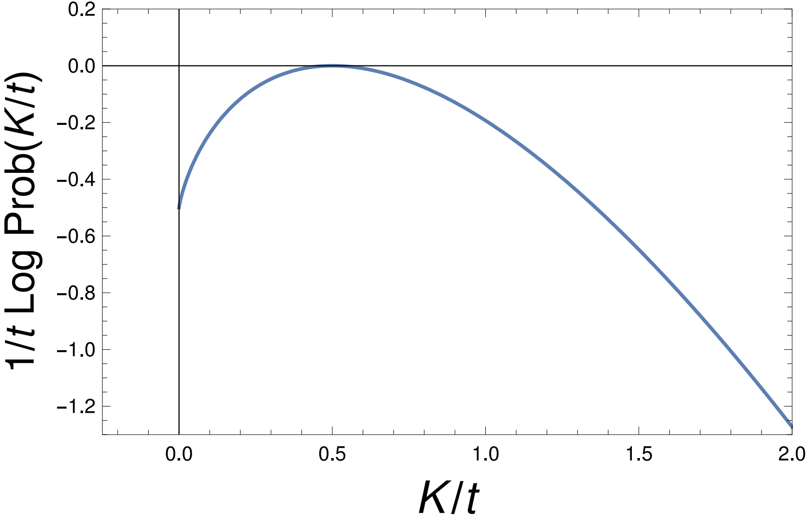
# How to perform averages?

⋆ Mid-time ancestor distribution:

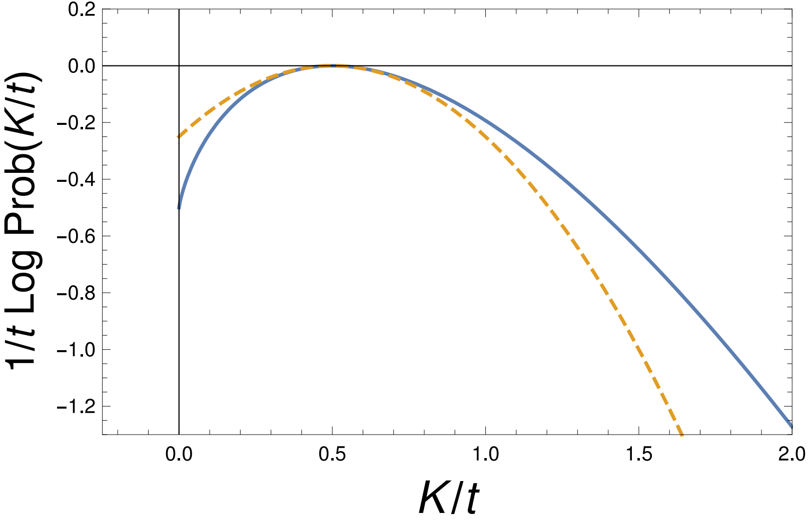
fraction of copies (at time $t_1$) which were in configuration $\mathcal{C}$, knowing that there are in configuration $\mathcal{C}_\mathrm{f}$ at final time $t_\mathrm{f}$:

$$p_\mathrm{anc}(\mathcal{C},t_1;\mathcal{C}_\mathrm{f},t_\mathrm{f}) = \frac{\langle N_\mathrm{nc}(\mathcal{C}_\mathrm{f},t_\mathrm{f}|\mathcal{C},t_1)\rangle_s}{\sum_{\mathcal{C}'}\langle N_\mathrm{nc}(\mathcal{C}_\mathrm{f},t_\mathrm{f}|\mathcal{C}',t_1)\rangle_s} \underset{t_{\mathrm{f},1}\to\infty}{\sim} \langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle = p_\mathrm{ave}(\mathcal{C})$$

**The “ancestor statistics” of a configuration $\mathcal{C}_\mathbf{f}$ is thus independent (far enough in the past) of the configuration $\mathcal{C}_\mathbf{f}$.**




$$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$$

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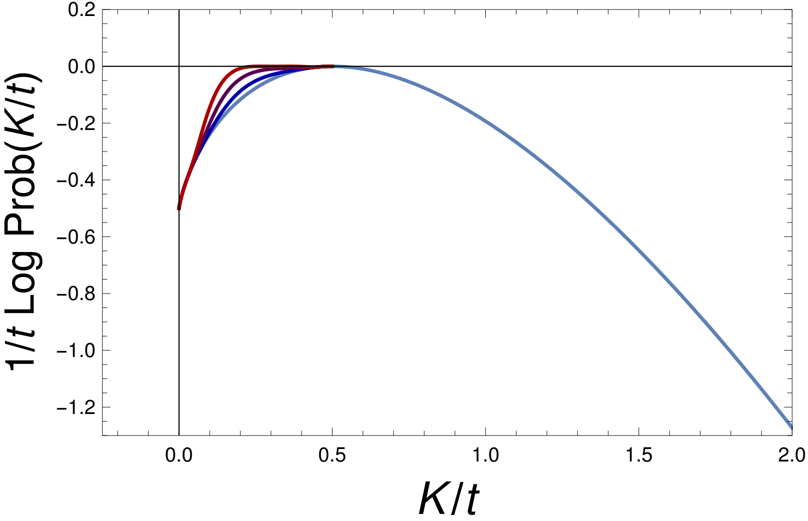


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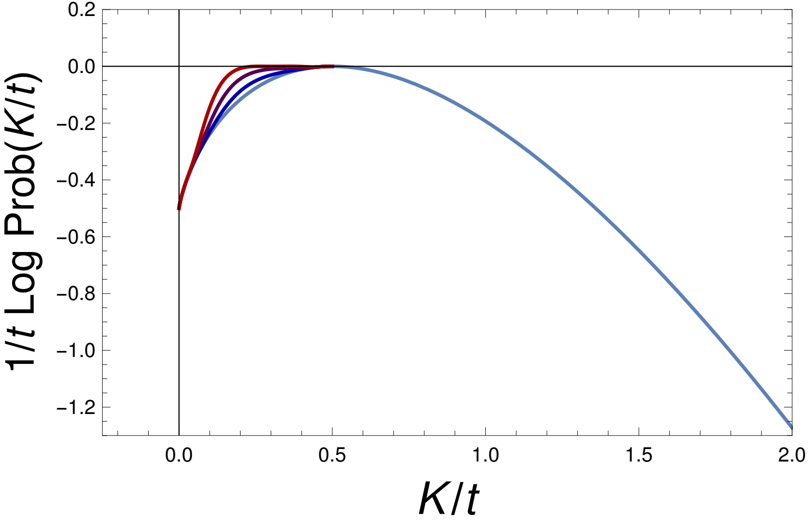
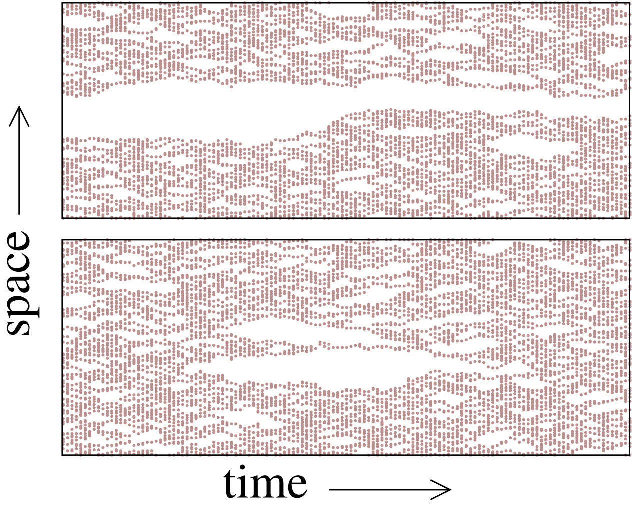
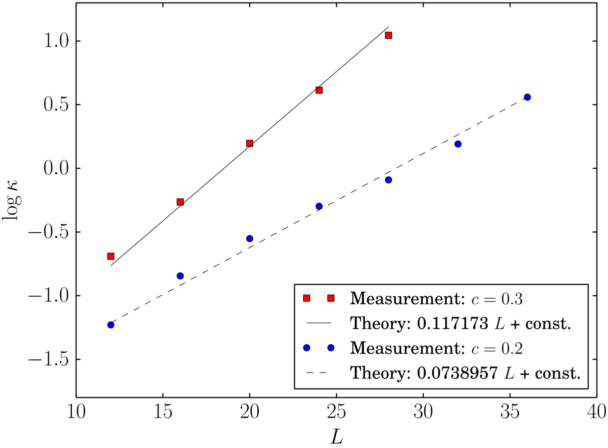



$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.

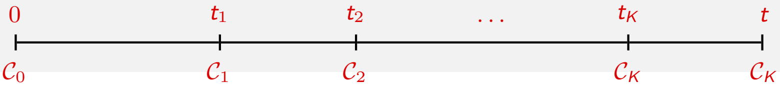



[Merolle, Garrahan and Chandler, 2005]




Exponential divergence of the susceptibility

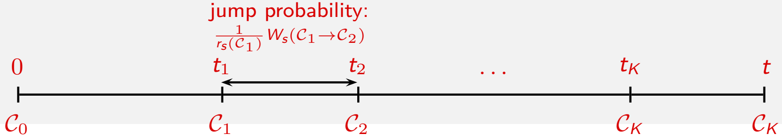
# Explicit construction (1/3)




## Probability-preserving contribution

$$\partial_t \hat{P}(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W_s(\mathcal{C} \to \mathcal{C}')\hat{P}(\mathcal{C},t)}_{\text{loss term}} \Big\}$$

# Explicit construction (1/3)




## Which configurations will be visited?

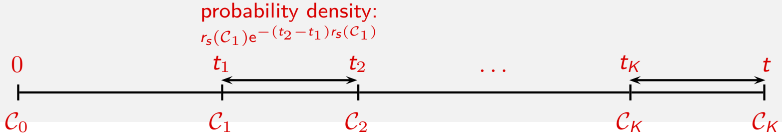
Configurational part of the trajectory: $\mathcal{C}_0 \to \ldots \to \mathcal{C}_K$

$$\mathrm{Prob}\{\mathrm{hist}\} = \prod_{n=0}^{K-1} \frac{W_s(\mathcal{C}_n \to \mathcal{C}_{n+1})}{r_s(\mathcal{C}_n)}$$

where

$$r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}')$$

# Explicit construction (2/3)

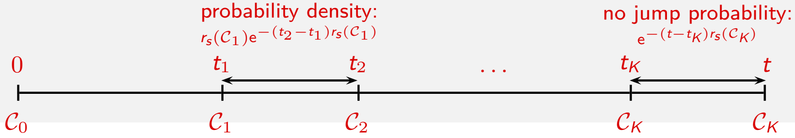



**When shall the system jump from one configuration to the next one?**

- probability density for the time interval $t_n - t_{n-1}$

$$r_s(\mathcal{C}_{n-1})\mathrm{e}^{-(t_n-t_{n-1})r_s(\mathcal{C}_{n-1})}$$

# Explicit construction (2/3)

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- probability density for the time interval $t_n - t_{n-1}$

$$r_s(\mathcal{C}_{n-1})\mathrm{e}^{-(t_n-t_{n-1})r_s(\mathcal{C}_{n-1})}$$

- probability not to leave $\mathcal{C}_K$ during the time interval $t - t_K$

$$\mathrm{e}^{-(t-t_K)r_s(\mathcal{C}_K)}$$

# Explicit construction (3/3)

$$\partial_t \hat{P}(\mathcal{C},s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}',s) - r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{modified dynamics}} \;+\; \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C},s)}_{\text{cloning term}}$$

**How to take into account loss/gain of probability?**

- handle a large number of copies of the system
- implement a selection rule: on a time interval $\Delta t$ a copy in config $\mathcal{C}$ is replaced by $e^{\Delta t\,\delta r_s(\mathcal{C})}$ copies
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

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**How to take into account loss/gain of probability?**

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- implement a selection rule: on a time interval $\Delta t$
  a copy in config $\mathcal{C}$ is replaced by $\lfloor e^{\Delta t\, \delta r_s(\mathcal{C})} + \varepsilon \rfloor$ copies, $\epsilon \sim [0, 1]$
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# Explicit construction (3/3)

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## Biological interpretation

- copy in configuration $\mathcal{C} \equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s \equiv$ **mutations**
- cloning at rates $\delta r_s \equiv$ **selection** rendering atypical histories typical